ON A "HAMILTONIAN PATH-INTEGRAL" DERIVATION OF THE SCHRODINGER EQUATION (Spectral-scattering theory and related topics)

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ON A "HAMILTONIAN PATH-INTEGRAL" DERIVATION OF THE SCHRÖDINGER EQUATION

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§1. PROBLEM AND RESULT

Problem: Construct a parametrix which exhibits clearly how quantities from Hamiltonian mechanics are related to quantum mechanics: ("**Hamiltonian path-integral quantization**" in $L^2(\mathbb{R}^m)$)

$$\begin{cases} \dfrac{\hbar}{i}\dfrac{\partial u(t,x)}{\partial t} + \mathbb{H}\left(t,x,\dfrac{\hbar}{i}\dfrac{\partial}{\partial x}\right)u(t,x) = 0, \\ u(0,x) = \underline{u}(x) \end{cases} \tag{1}$$

with

$$\mathbb{H}\left(t,x,\frac{\hbar}{i}\frac{\partial}{\partial x}\right) = \frac{1}{2}\sum_{j=1}^{m}\left(\frac{\hbar}{i}\frac{\partial}{\partial x_j} - A_j(t,x)\right)^2 + V(t,x).$$

Assumptions:

(A) $A_j(t,x) \in C^\infty(\mathbb{R}\times\mathbb{R}^m)$, real-valued and there exists $\epsilon > 0$ such that

$$|\partial_x^\alpha B_{jk}(t,x)| \le C_\alpha (1+|x|)^{-1-\epsilon} \ \text{ for } \ |\alpha| \ge 1,$$
$$|\partial_x^\alpha A_j(t,x)| + |\partial_x^\alpha \partial_t A_j(t,x)| \le C_\alpha \ \text{ for } \ |\alpha| \ge 1$$

where

$$B_{jk}(t,x) = \frac{\partial A_j(t,x)}{\partial x_k} - \frac{\partial A_k(t,x)}{\partial x_j}.$$

(V) $V(t,x) \in C^\infty(\mathbb{R}\times\mathbb{R}^m)$, real-valued and for any compact interval I, there exists a constant $C_{\alpha I} > 0$ such that

$$\sup_{t\in I} |\partial_x^\alpha V(t,x)| \le C_{\alpha I} \ \text{ for } \ |\alpha| \ge 2.$$

Outline of the strategy of quantization:

(I) Let $H(t,x,\xi)$ be given (e.g. the complete symbol of $\mathbb{H}(t,x,-i\hbar\partial_x)$). Solve

$$\begin{cases} \dot{x}(t) = \partial_\xi H(t,x(t),\xi(t)), \\ \dot{\xi}(t) = -\partial_x H(t,x(t),\xi(t)). \end{cases} \tag{2}$$

(II) Under Assumptions (A) and (V), construct a phase function $S(t,s,x,\xi)$ (Hamilton-Jacobi equation):

$$\begin{cases} \partial_t S(t,s,x,\xi) + H(t,x,\partial_x S(t,s,x,\xi)) = 0, \\ S(s,s,x,\xi) = x\cdot\xi. \end{cases} \tag{3}$$

Then, $D(t,s,x,\xi) = \det(\partial^2_{x_j\xi_k} S(t,s,x,\xi))$ satisfies the continuity equation:

$$\begin{cases} \partial_t D(\cdot) + \partial_x\big[D(\cdot)\partial_\xi H(t,x,\partial_x S(t,s,x,\xi))\big] = 0, \\ D(s,s,x,\xi) = 1. \end{cases} \tag{4}$$

(III) Define a Fourier Integral Operator on $\mathbb{R}^m$ as

$$E(t,s)u(x) = c_m \int_{\mathbb{R}^m} d\xi\, D^{1/2}(t,s,x,\xi)\, e^{i\hbar^{-1}S(t,s,x,\xi)}\hat{u}(\xi) \tag{5}$$

where $c_m = (2\pi\hbar)^{-m/2}$ and

$$\hat{u}(\xi) = c_m \int_{\mathbb{R}^m} dx\, e^{-i\hbar^{-1}x\cdot\xi} u(x).$$

(IV) This operator gives a **good parametrix** for (1) on $L^2(\mathbb{R}^m)$, by virtue of (3) and (4).

For a subdivision Δ of (s,t), put

$$\Delta : t_0 = s < t_1 < \cdots < t_{\ell-1} < t_\ell = t, \quad \delta(\Delta) = \max_{j=1,\cdots,\ell} |t_j - t_{j-1}|,$$
$$E(\Delta|t,s)u = E(t,t_{\ell-1})E(t_{\ell-1},t_{\ell-2})\cdots E(t_1,s).$$

Main Theorem. *Fix $T>0$ arbitrarily. Assume (A) and (V). $(t,s)\in[-T,T]^2$.*

(0) $\{E(\Delta|t,s)\}$ converges to $\mathbb{U}(t,s)$ when $\delta(\Delta)\to 0$ in $L^2(\mathbb{R}^m)$ s.t.

$$\|E(\Delta|t,s) - \mathbb{U}(t,s)\| \le C\delta(\Delta).$$

(1) $\mathbb{U}(t,s) \in \mathbb{B}(L^2(\mathbb{R}^m) : L^2(\mathbb{R}^m))$.

(2) $\mathbb{U}(t,s)$ *is* $L^2(\mathbb{R}^m)$*-valued continuous and*

$$\begin{cases} \mathbb{U}(s,s) = I, \\ \mathbb{U}(t,s)\mathbb{U}(s,r) = \mathbb{U}(t,r). \end{cases}$$

(3) If $u \in C_0^\infty(\mathbb{R}^m)$, $\mathbb{U}(t,s)u$ *satisfies*

$$\begin{cases} \frac{\hbar}{i}\frac{\partial}{\partial t}\mathbb{U}(t,s)u + \mathbb{H}\Big(t,x,\frac{\hbar}{i}\frac{\partial}{\partial x}\Big)\mathbb{U}(t,s)u = 0, \\ \frac{\hbar}{i}\frac{\partial}{\partial s}\mathbb{U}(t,s)u - \mathbb{U}(t,s)\mathbb{H}\Big(s,x,\frac{\hbar}{i}\frac{\partial}{\partial x}\Big)u = 0. \end{cases}$$

§2. Feynman's heuristic argument

Consider the following initial value problem:

$$(*) \qquad \begin{cases} i\hbar\frac{\partial}{\partial t}u(x,t) = -\frac{\hbar^2}{2}\Delta u(x,t) + V(x)u(x,t), \\ u(x,0) = \underline{u}(x). \end{cases}$$

Here, the Hamiltonian is given formally as

$$H = -\frac{\hbar^2}{2}\Delta + V(\cdot) = H_0 + V, \quad \Delta = \sum_{j=1}^m \frac{\partial^2}{\partial x_j^2}.$$

Assuming H is essentially selfadjoint in $L^2(\mathbb{R}^m)$, by Stone's theorem, we have the solution of (*) as

$$u(x,t) = (e^{-\frac{i}{\hbar}tH}\underline{u})(x).$$

On the other hand, by the Lie-Trotter-Kato product formula, we have

$$e^{-\frac{i}{\hbar}tH} = \operatorname*{s-lim}_{k\to\infty}\left(e^{-\frac{i}{\hbar}\frac{t}{k}V}e^{-\frac{i}{\hbar}\frac{t}{k}H_0}\right)^k.$$

If the initial data $\underline{u}$ belongs to $\mathcal{S}(\mathbb{R}^m)$, we get

$$(e^{-\frac{i}{\hbar}tH_0}\underline{u})(x) = (2\pi i\hbar t)^{-m/2}\int_{\mathbb{R}^m} dy\, e^{i(x-y)^2/(2\hbar t)}\underline{u}(y).$$

Therefore,

$$(e^{-\frac{i}{\hbar}tH}\underline{u})(x) = \int dy\, F(t,x,y)\underline{u}(y),$$

with

$$F(t,x,y) = \operatorname*{s-lim}_{k\to\infty} (2\pi i\hbar t)^{-km/2} \int \cdots \int dx^{(1)} \cdots dx^{(k-1)} e^{\frac{i}{\hbar} S_t(x, x^{(k-1)}, \cdots, x^{(1)}, y)}.$$

Here, we put $x^{(k)} = x,\ x^{(0)} = y$,

$$S_t(x^{(k)}, \ldots, x^{(0)}) = \sum_{j=1}^{k} \left[\frac{1}{2} \frac{(x^{(j)} - x^{(j-1)})^2}{(t/k)^2} - V(x^{(j)}) \right] \frac{t}{k}.$$

Feynman's interpretation: Let

$$C_{t,x,y} = \{\gamma(\cdot) \in AC([0,t] : \mathbb{R}^m) \mid \gamma(0) = y, \gamma(t) = x\}.$$

For any path $\gamma \in C_{t,x,y}$, $S_t(x^{(k)}, \ldots, x^{(0)})$ is regarded as the Riemann sum for the classical action $S_t(\gamma)$, i.e.

$$S_t(\gamma) = \int_0^t L(\gamma(\tau), \dot{\gamma}(\tau)) d\tau = \lim_{k\to\infty} S_t(x^{(k)}, \ldots, x^{(0)}),$$

where

$$L(\gamma, \dot{\gamma}) = \frac{1}{2}\dot{\gamma}^2 - V(\gamma) \in C^\infty(T\mathbb{R}^m)$$

When $k \to \infty$, the 'limit' of the measure $dx^{(1)} \cdots dx^{(k-1)}$ is denoted by

$$d_F\gamma = \prod_{0<\tau<t} d\gamma(\tau)$$

and considered as the 'measure' on the path space $C_{t,x,y}$ (See S.A. Albeverio & R.J. Hoegh-Krohn [1]).

Feynman's conclusion:

$$F(t,x,y) = \int_{C_{t,x,y}} d_F\gamma\, e^{\frac{i}{\hbar}\int_0^t L(\gamma(\tau), \dot{\gamma}(\tau)) d\tau}.$$

On the other hand, it is proved unfortunately that there exists no non-trivial 'Feynman measure' on ∞-dimensional spaces.

Problem 1. Give a meaning to

$$\int d_F\gamma\, e^{i\hbar^{-1}\int_0^t L(\gamma(\tau), \dot{\gamma}(\tau)) d\tau}.$$

A partial solution of this problem is presented by Fujiwara [12], when $|\partial_x^\alpha V(x)| \leq C_\alpha$ for $|\alpha| \geq 2$.

Problem 2. As a Hamiltonian counter part of above, how do we define

$$\iint d_F x d_F \xi \, e^{i\hbar^{-1}\int_0^t H(x(\tau),\xi(\tau))d\tau} \, ?$$

See, Inoue [17].

Method of characteristics as quantization

On the region Ω in $\mathbb{R}^{m+1}$, we consider the following initial value problem:

$$\begin{cases} \dfrac{\partial}{\partial t}u(t,q) + \displaystyle\sum_{j=1}^m a_j(t,q)\frac{\partial}{\partial q_j}u(t,q) = b(t,q)u(t,q) + f(t,q), \\ u(\underline{t},q) = \underline{u}(q). \end{cases}$$

Corresponding characteristics are given by

$$\begin{cases} \dfrac{d}{dt}q_j(t) = a_j(t,q(t)), \\ q_j(\underline{t}) = \underline{q}_j \quad (j = 1, \cdots, m). \end{cases}$$

When this is solved nicely, we denote them as

$$q(t) = q(t,\underline{t};\underline{q}) = (q_1(t), \cdots, q_m(t)) \in \mathbb{R}^m.$$

Following theorem is well-known.

Theorem. *Let $a_j \in C^1(\Omega:\mathbb{R})$ and $b, f \in C(\Omega:\mathbb{R})$. For any point $(\underline{t},\underline{q}) \in \Omega$, we asume that $\underline{u}$ is C^1 in a neighbourhood of $\underline{q}$.*

Then, in a neighbourgood of $(\underline{t},\underline{q})$, there exists uniquely a solution $u(t,q)$. More precisely, putting

$$U(t,\underline{q}) = e^{\int_{\underline{t}}^t d\tau\, B(\tau,\underline{q})}\left\{\int_{\underline{t}}^t ds\, e^{-\int_{\underline{t}}^s d\tau\, B(\tau,\underline{q})}F(s,\underline{q}) + \underline{u}(\underline{q})\right\},$$

solution is represented by

$$u(t,\bar{q}) = U(t, y(t,\underline{t};\bar{q}))$$

where $B(t,\underline{q}) = b(t,q(t,\underline{t};\underline{q}))$, $F(t,\underline{q}) = f(t,q(t,\underline{t};\underline{q}))$ and $\underline{q} = y(t,\underline{t};\bar{q})$ is a inverse function defined from $\bar{q} = q(t,\underline{t};\underline{q})$.

We apply above theorem to the simplest case:

$$\begin{cases} i\hbar\dfrac{\partial}{\partial t}u(t,q) = a\dfrac{\hbar}{i}\dfrac{\partial}{\partial q}u(t,q) + bqu(t,q), \\ u(0,q) = \underline{u}(q). \end{cases}$$

From the right-hand side of above, we define a Hamiltonian as follows (more precisely, Weyl symbol should be considered):

$$H(q,p) = e^{-i\hbar^{-1}qp}\Big(a\frac{\hbar}{i}\frac{\partial}{\partial q} + bq\Big)e^{i\hbar^{-1}qp} = ap + bq.$$

The classical mechanics associated to that Hamiltonian is given by

$$\begin{cases} \dot{q}(t) = H_p = a, \\ \dot{p}(t) = -H_q = -b \end{cases} \text{with } \begin{pmatrix} q(0) \\ p(0) \end{pmatrix} = \begin{pmatrix} \underline{q} \\ \underline{p} \end{pmatrix}$$

which is readily solved as

$$q(s) = \underline{q} + as, \quad p(s) = \underline{p} - bs.$$

From above theorem, putting $\underline{t} = 0$, we get readily that

$$U(t,\underline{q}) = \underline{u}(\underline{q})e^{-i\hbar^{-1}(b\underline{q}t + 2^{-1}abt^2)}.$$

As the inverse function of $\bar{q} = q(t,\underline{q})$ is given by$\underline{q} = y(t,\bar{q}) = \bar{q} - at$, we get

$$u(t,\bar{q}) = U(t,\underline{q})|_{\underline{q}=y(t,\bar{q})} = \underline{u}(\bar{q} - at)e^{-i\hbar^{-1}(b\bar{q}t - 2^{-1}abt^2)}.$$

Another point of view: Put

$$S_0(t,\underline{q},\underline{p}) = \int_0^t ds\,[\dot{q}(s)p(s) - H(q(s),p(s))] = -b\underline{q}t - 2^{-1}abt^2,$$

$$S(t,\bar{q},\underline{p}) = \underline{q}\,\underline{p} + S_0(t,\underline{q},\underline{p})|_{\underline{q}=y(t,\bar{q})} = \bar{q}\underline{p} - a\underline{p}t - b\bar{q}t + 2^{-1}abt^2.$$

$S(t,\bar{q},\underline{p})$ satisfies the Hamilton-Jacobi equation.

$$\begin{cases} \dfrac{\partial}{\partial t}S + H(\bar{q},\partial_{\bar{q}}S) = 0, \\ S(0,\bar{q},\underline{p}) = \bar{q}\,\underline{p}. \end{cases}$$

On the other hand, the van Vleck determinant is

$$D(t,\bar{q},\underline{p}) = \frac{\partial^2 S(t,\bar{q},\underline{p})}{\partial\bar{q}\partial\underline{p}} = 1.$$

This quantity satisfies the continuity equation:

$$\begin{cases} \dfrac{\partial}{\partial t}D + \dfrac{1}{2}\partial_{\bar{q}}(DH_p) = 0 \quad \text{where } H_p = \dfrac{\partial H}{\partial p}(\bar{q}, \dfrac{\partial S}{\partial \bar{q}}), \\ D(0,\bar{q},\underline{p}) = 1. \end{cases}$$

As an interpretation of Feynman's idea, we regard that the transition from classical to quantum is to study the following quantity or the one represented by this (the term "quantization" is not so well-defined mathematically):

$$u(t,\overline{q}) = (2\pi\hbar)^{-1/2} \int_{\mathbb{R}} d\underline{p}\, D^{1/2}(t,\overline{q},\underline{p}) e^{i\hbar^{-1}S(t,\overline{q},\underline{p})} \underline{\hat{u}}(\underline{p}).$$

That is, in our case at hand, we should study the quantity defined by

$$\begin{aligned} u(t,\overline{q}) &= (2\pi\hbar)^{-1/2} \int_{\mathbb{R}} d\underline{p}\, e^{i\hbar^{-1}S(t,\overline{q},\underline{p})} \underline{\hat{u}}(\underline{p}) \\ &= (2\pi\hbar)^{-1} \iint_{\mathbb{R}^2} d\underline{p} d\underline{q}\, e^{i\hbar^{-1}(S(t,\overline{q},\underline{p}) - \underline{q}\,\underline{p})} \underline{u}(\underline{q}) = \underline{u}(\overline{q} - at) e^{i\hbar^{-1}(-b\overline{q}t + 2^{-1}abt^2)}. \end{aligned}$$

[Problem] Can we extend the above argument to a system of PDE? For example, Dirac, Weyl or Pauli equations, quantum mechanical equations with spin. See, Inoue [17-19] and Inoue & Maeda [21].

§3. Composition formulas.

Now, we put

$$\hat{H}^W(x, D_x^\hbar) = c_m^2 \int_{\mathbb{R}^{2m}} d\xi\, dx' e^{i\hbar^{-1}(x-x')\cdot\xi} H(\frac{x+x'}{2}, \xi) u(x'),$$

$$F(a,\phi)u(x) = c_m \int_{\mathbb{R}^m} d\xi\, a(x,\xi) e^{i\hbar^{-1}\phi(x,\xi)} \hat{u}(\xi).$$

Theorem. *For suitablly given $a(x,\xi)$, $\phi(x,\xi)$, $H(x,\xi)$, we have the following:*

(1) There exists $c_L = c_L(x,\eta) \in C^\infty(\mathbb{R}^{2m})$ s.t.
$\hat{H}^W(x, D_x^\hbar) F(a,\phi) = F(c_L, \phi)$ with

$$c_L = Ha - i\hbar\Big\{\partial_{\xi_j} H \cdot \partial_{x_j} a + \frac{1}{2}\Big(\partial^2_{x_j\xi_j} H + \partial^2_{x_j x_k}\phi \cdot \partial^2_{\xi_k\xi_j} H\Big) a\Big\} + r_L.$$

Here, $H = H(x, \partial_x\phi)$, $\phi = \phi(x,\eta)$ and $r_L = r_L(x,\eta)$,

$$r_L(x,\eta) = -\frac{\hbar^2}{2} \partial^2_{\xi_k\xi_j} H(x, \partial_x\phi(x,\eta))\, \partial^2_{x_j x_k} a(x,\eta).$$

(2) There exists $c_R = c_R(x,\xi) \in C^\infty(\mathbb{R}^{2m})$ s.t.
$F(a,\phi)\hat{H}^W(x, D_x^\hbar) = F(c_R, \phi)$ with

$$c_R = aH - i\hbar\Big\{\partial_{\xi_j} a \cdot \partial_{x_j} H + \frac{1}{2} a\Big(\partial^2_{\xi_j x_j} H + \partial^2_{\xi_j\xi_k}\phi \cdot \partial^2_{x_k x_j} H\Big)\Big\} + r_R.$$

Here, $H = H(\partial_\xi\phi(x,\xi), \xi)$, $c_R = c_R(x,\xi)$, $a = a(x,\xi)$ and $\phi = \phi(x,\xi)$,

$$r_R(x,\xi) = r_{Ri}^{(1)}(x,\xi)\xi_i + r_R^{(0)}(x,\xi).$$

§4. Properties of parametrix

Proposition. *Assume (A), (V) and $|t-s| \le \delta_1$. Then, for any $\hat{u} \in C_0^\infty(\mathbb{R}^m)$, there exists a constant C such that*

$$\|E(t,s)u\| \le C\|u\|.$$

Proposition. *(1) For each $u \in L^2(\mathbb{R}^m)$, we have*

$$\operatorname*{s-lim}_{|t-s|\to 0} E(t,s)u = u \qquad in \quad L^2(\mathbb{R}^m).$$

(2) If we set $E(s,s) = I$, then the correspondence $(s,t) \to E(t,s)u$ gives a strongly continuous function with values in $L^2(\mathbb{R}^m)$.

Proposition. *Let $u \in C_0^\infty(\mathbb{R}^m)$.*

$$\frac{\hbar}{i}\frac{\partial}{\partial t}E(t,s)u(x) = -\hat{H}^W(t,x,D_x)E(t,s)u(x) + G(t,s)u(x),$$
$$\|G(t,s)u\| \le C\hbar^2|t-s|\|u\|.$$

Proof. Using the Hamilton-Jacobi and the continuity equations with the product formula, we get

$$\frac{\hbar}{i}(\mu_t + i\hbar^{-1}S_t\,\mu) = \frac{\hbar}{i}(\cdots) - \mu\,H$$
$$= -[\text{amplitude part of the "symbol" of } (\hat{H}^W(t,x,D_x)E(t,s))] - r_L.$$

$r_L = -\frac{\hbar^2}{2}\Delta_x\mu(t,s,x,\xi)$, $\mu = \mu(\cdots)$ and $S = S(\cdots)$, $H = H(x, \partial_x S(t,s,x,\xi))$.

$$|\partial_x^\alpha \partial_\xi^\beta r_L(t,s,x,\xi)| \le C_{\alpha\beta}\hbar^2|t-s|.$$

Use Calderon-Vaillancourt's theorem. □

Proposition. *Let $|||u|||_1 = \|\langle x\rangle u\| + \|\partial_x u\|$.*

$$\frac{\hbar}{i}\frac{\partial}{\partial s}E(t,s)u(x) = E(t,s)\hat{H}^W(s,x,D_x)u(x) + \tilde{G}(t,s)u(x),$$
$$\|\tilde{G}(t,s)u\| \le C\hbar^2|t-s|\,|||u|||_1$$

Remark. The above estimate is crucial why we can't proceed as in the Lagarngian formalism. But in case $A_i(t,x) = a_{ij}(t)x_j$, we have

$$\|\tilde{G}(t,s)u\| \le C\hbar^2|t-s|\|u\|.$$

Proceeding as in Fujiwara, we have

Propositon.

$$(**) \qquad \|(E(t,s)E(s,r)-E(t,r))u\| \le C\hbar(|t-s|^2+|s-r|^2)|||u|||_1,$$

$$(***) \qquad \|(E(s,t)^*E(s,r)-E(t,r))u\| \le C\hbar(|t-s|^2+|s-r|^2)\|u\|.$$

Corollary. *From (***), we have*

$$\|E(t,s)\| \le e^{C\hbar|t-s|^2}.$$

§5. Composition of FIOs

Let $|t-s|+|s-r|$ be sufficiently small. We want to calculate the quantity $\|E(t,s)E(s,r)u-E(t,r)u\|$ directly without using the adjoint operation.

Lemma. *For any x,ξ, there exists a unique solution (X,Ξ) of*

$$\begin{cases} X_j = \partial_{\xi_j}S(t,s,x,\Xi), \\ \Xi_j = \partial_{x_j}S(s,r,X,\xi). \end{cases}$$

$$|\partial_x^\alpha\partial_\xi^\beta(X_j-x_j)| \le C_{\alpha,\beta}(1+|x|+|\xi|)^{(1-|\alpha+\beta|)_+},$$
$$|\partial_x^\alpha\partial_\xi^\beta(\Xi_j-\xi_j)| \le C_{\alpha,\beta}(1+|x|+|\xi|)^{(1-|\alpha+\beta|)_+}.$$

Put $X=X(t,s,r,x,\xi)$, $\Xi=\Xi(t,s,r,x,\xi)$ and

$$\Phi(t,s,r,x,\xi) = S(t,s,x,\Xi)-X\Xi+S(s,r,X,\xi).$$

Lemma. *As we calculate easily*

$$\begin{cases} \dfrac{\partial}{\partial s}\Phi(t,s,r,x,\xi)=0, \\ \dfrac{\partial}{\partial t}\Phi(t,s,r,x,\xi) = -H(t,x,\partial_x\Phi(t,s,r,x,\xi)), \\ \dfrac{\partial}{\partial r}\Phi(t,s,r,x,\xi) = H(r,\partial_\xi\Phi(t,s,r,x,\xi),\xi), \end{cases}$$

we get

$$\Phi(t,s,r,x,\xi) = S(t,r,x,\xi).$$

Remark. $\Phi(t,s,r,x,\xi)$ is called a $\#$-product of $S(t,s,x,\xi)$ and $S(s,r,x,\xi)$, and which is denoted by $S(t,s,x,\cdot)\#S(s,r,\cdot,\xi)$.

Now, we have, as an oscillatory integral,

$$E(t,s)E(s,r)u(x) = c_m^3 \int_{\mathbb{R}^{3m}} d\eta\, dy\, d\xi\, \mu(t,s,x,\eta)\mu(s,r,y,\xi) \times e^{i\hbar^{-1}(S(t,s,x,\eta)-y\eta+S(s,r,y,\xi))}\,\hat{u}(\xi).$$

Using the change of variables

$$y = X + \tilde{y}, \quad \eta = \Xi + \tilde{\eta},$$

we have

$$E(t,s)E(s,r)u(x) - E(t,r)u(x) = c_m \int_{\mathbb{R}^m} d\xi\, b(t,s,r,x,\xi) e^{i\hbar^{-1}S(t,r,x,\xi)}\hat{u}(\xi)$$

with

$$b(t,s,r,x,\xi) = \Big[c_m^2 \int_{\mathbb{R}^{2m}} d\tilde{\eta}\, d\tilde{y}\, \mu(t,s,x,\Xi+\tilde{\eta})\mu(s,r,X+\tilde{y},\xi) \times e^{i\hbar^{-1}(R(t,s,r,x,\xi,\tilde{y},\tilde{\eta})-\tilde{y}\tilde{\eta})}\Big] - \mu(t,r,x,\xi),$$

$$S(t,s,x,\eta) - y\eta + S(s,r,y,\xi) - S(t,r,x,\xi) = -\tilde{y}\tilde{\eta} + R(t,s,r,x,\xi,\tilde{y},\tilde{\eta}).$$

Propositon. *[Taniguchi [29]]*

$$|\partial_x^\alpha \partial_\xi^\beta b(t,s,r,x,\xi)| \le C_{\alpha,\beta}(|t-s|^2 + |s-r|^2).$$

In spite of the estimate (**), we have

Corollary.

$$\|E(t,s)E(s,r)u - E(t,r)u\| \le C(|t-s|^2 + |s-r|^2)\|u\|.$$

§6. The comparison with two formalisms

Theorem. *[Lagrangian formulation] A parametrix of the initial value problem (1) is given by*

$$\tilde{E}(t,s)u(x) = \tilde{c}_m \int dy\, \tilde{\mu}(t,s,x,y) e^{i\hbar^{-1}\tilde{S}(t,s,x,y)}u(y).$$

$\tilde{c}_m = (2\pi i\hbar)^{-m/2} = c_m e^{-m\pi i/4}$, $\tilde{S}(t,s) = \tilde{S}(t,s,x,y)$ satisfies

$$\begin{cases} \partial_t \tilde{S}(t,s) + H(t,x,\partial_x \tilde{S}(t,s)) = 0, \\ \lim_{t\to s} (t-s)\tilde{S}(t,s) = \frac{1}{2}|x-y|^2, \end{cases}$$

and $\tilde{\mu}(t,s) = \tilde{\mu}(t,s,x,y)$ satisfies

$$\begin{cases} \partial_t \tilde{\mu}(t,s) + \partial_{x_j}\tilde{\mu}(t,s) H_{\xi_j}(t,x,\partial_x \tilde{S}(t,s)) + \frac{1}{2}\tilde{\mu}(t,s)\frac{\partial}{\partial x_j} H_{\xi_j}(t,x,\partial_x \tilde{S}(t,s)) = 0, \\ \lim_{t\to s} (t-s)^{m/2}\tilde{\mu}(t,s) = 1. \end{cases}$$

Corollary.

$$\begin{aligned} &\partial_s \tilde{S}(t,s) - H(s,y,-\partial_y \tilde{S}(t,s)) = 0, \\ &\partial_s \tilde{\mu}(t,s) - \partial_{y_k}\tilde{\mu}(t,s) H_{\xi_k}(s,y,-\partial_y \tilde{S}(t,s)) \\ &\qquad\qquad - \frac{1}{2}\tilde{\mu}(t,s)\frac{\partial}{\partial y_k} H_{\xi_k}(s,y,-\partial_y \tilde{S}(t,s)) = 0. \end{aligned}$$

Here, we put

$$\tilde{\mu}(t,s,x,y) = \left[\det\left(\frac{\partial^2 \tilde{S}(t,s,x,y)}{\partial x_j \partial y_k}\right)\right]^{1/2}.$$

Proposition.

$$\begin{aligned} &\frac{\partial}{\partial t}\tilde{E}(t,s)u + \mathbb{H}(t,x,D_x^\hbar)\tilde{E}(t,s)u = \tilde{G}_L(t,s)u, \\ &\qquad \|\tilde{G}_L(t,s)u\| \le C\hbar^2|t-s|\|u\|. \end{aligned}$$

Proposition.

$$\begin{aligned} &\frac{\partial}{\partial s}\tilde{E}(t,s)u - \tilde{E}(t,s)\mathbb{H}(s,y,D_y^\hbar)u = \tilde{G}_R(t,s)u, \\ &\qquad \|\tilde{G}_R(t,s)u\| \le C\hbar^2|t-s|\|u\|. \end{aligned}$$

Proof. By the integration by parts under the oscillatory integral sign, we have

$$\begin{aligned} &\int dy\, \tilde{\mu}(t,s,x,y)e^{i\hbar^{-1}\tilde{S}(t,s,x,y)}\mathbb{H}(s,y,D_y^\hbar)u(y) \\ &\quad = \int dy \left[\frac{1}{2}\Big(\frac{\hbar}{i}\frac{\partial}{\partial y_j} + A_j(s,y)\Big)^2 - V(s,y)\right]\left(\tilde{\mu}(t,s,x,y)e^{i\hbar^{-1}\tilde{S}(t,s,x,y)}\right)u(y). \quad \square \end{aligned}$$

From these propositions, we have

Proposition.

$$\|\tilde{E}(t,s)\tilde{E}(s,r) - \tilde{E}(t,r)\| \le C\hbar(|t-s|^2 + |s-r|^2),$$
$$\|\tilde{E}(s,t)^*\tilde{E}(s,r) - \tilde{E}(t,r)\| \le C\hbar(|t-s|^2 + |s-r|^2).$$

The difference.

(1) $\hat{H}^W(t,x,D_x^\hbar)$ is derived from $H(t,x,\xi)$ using the Fourier transformation, while $\mathbb{H}(t,x,D_x^\hbar)$ is used as a given operator without considering from where it stemms.

(2) In the Lagrangian formulation, the time reversing and taking the adjoint are rather nicely related.

To show this, we have

Proposition. *Under Assumptions (A) and (V), we have*

$$\tilde{S}(t,s,x,y) = -\tilde{S}(s,t,y,x).$$

Therefore, we have

Corollary.

$$\tilde{\mu}(t,s,x,y) = \tilde{\mu}(t,s,y,x) = (-1)^{m/2}\tilde{\mu}(s,t,y,x).$$

Now, we have

Proposition. *Under these circumstance, we have*

$$\tilde{E}(t,s)^* = \tilde{E}(s,t).$$

Though in the Hamiltonian formulation, this relation does not seem to hold in general, we have

Proposition.

$$\|E(t,s)^* - E(s,t)\| \le C|t-s|^2.$$

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